2-Methoxyethyl acetoacetate

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Model Performance

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Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.93	22.5	0.93	22.1	0.93	22.1	

Model Results

Predicted value: 203 °C

Global applicability domain: Inside

Local applicability domain index: 6.48e-01

Confidence level: 7.82e-01

Nearest Neighbors from the Training Set

Image not found

2-Chloroethyl acetoacetate

Measured: 198 Predicted: 199

Image not found

Ethyl isobutyrylacetate

Measured: 173 Predicted: 194